

3-Bromophenylurea
2989-98-2 | DTXSID70184008

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.93e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.73e-01

Confidence level: 3.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Naphthalene, 1,2,4,7-tetrachloro-</div> <div>Measured: 3.45e-10</div> <div>Predicted: 1.23e-05</div>	<div>Image not found</div> <div>Pirimiphos-ethyl</div> <div>Measured: 2.00e-06</div> <div>Predicted: 2.79e-05</div>	<div>Image not found</div> <div>o-Vinyltoluene</div> <div>Measured: 1.71e-05</div> <div>Predicted: 1.93</div>
<div>Image not found</div> <div>1,4-Dimethylnaphthalene</div> <div>Measured: 1.63e-05</div> <div>Predicted: 6.77e-03</div>	<div>Image not found</div> <div>1-Undecene</div> <div>Measured: 2.46e-03</div> <div>Predicted: 3.07e-01</div>	